

Fresnel aperture diffraction: a phase-sensitive probe for superconducting pairing symmetry

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Fresnel single aperture diffraction (FSAD) is proposed as a phase-sensitive probe for pairing symmetry and Fermi surface of a superconductor. We consider electrons injected, through a small aperture, into a thin superconducting (SC) layer. It is shown that in case of SC gap symmetry $\Delta(-k_x, \mathbf{k}_{\parallel}) = \Delta(k_x, \mathbf{k}_{\parallel})$ with k_x and \mathbf{k}_{\parallel} respectively the normal and parallel component of electron Fermi wavevector, quasiparticle FSAD pattern developed at the image plane is zeroth-order minimum if $k_x x = n\pi$ (n is an integer and x is SC layer thickness). In contrast, if $\Delta(-k_x, \mathbf{k}_{\parallel}) = -\Delta(k_x, \mathbf{k}_{\parallel})$, the corresponding FSAD pattern is zeroth-order maximum. Observable consequences are discussed for iron-based superconductors of complex multi-band pairings.

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Recently high- T_c superconductivity has been observed in several classes of Fe-pnictide materials [1, 2]. One key issue for understanding the superconductivity of pnictides lies on the pairing symmetry of the Cooper pairs. A conclusive observation of the pairing symmetry remains unsettled to which both nodal and nodeless order parameters were reported in recent experiments, however. ARPES measurements indicated clearly a nodeless gap at all points on Fermi surfaces (FS) [3, 4] and magnetic penetration depth measurements further suggested the gap being possibly in the s^{\pm} state [5–7]. The s^{\pm} state is currently a promising pairing candidate for iron pnictides, which changes sign between α and β bands and can be naturally explained by the spin fluctuation mechanism [7–9]. On the contrary, the scanning SQUID microscopy measurements seemed to exclude the spin-triplet pairing states and suggested the order parameter having well-developed nodes [10]. In addition, NMR experiments were also in favor of nodal SC order parameters [11, 12]. For phase sensitive experiments, one point-contact spectroscopy reported was in favor of a nodal gap [13], while the other reported was in favor of a nodeless gap [14].

The complex pairing symmetry of these materials suggests that the pairing mechanism is likely non-universal and may depend strongly on the fine details of the band structures. With this regard, some possible experiments were proposed to elucidate these issues [15–17]. In this paper, Fresnel single aperture diffraction (FSAD) of electrons is proposed as a phase-sensitive probe for studying the SC pairing symmetry. Of particular interest, it is suggested that FSAD could be very useful for studying the iron-pnictide superconductors of complex multiple FS pairings. It will be shown that large Z (effective potential barrier) zeroth-order FSAD pattern is sensitive to both the SC phase and the probing direction and thus can give an unambiguous signal to distinguish different pairing symmetries among different FSs.

Fig. 1 sketches the proposed apparatus of a FSAD experiment. A substrate layer, made of a good conduc-

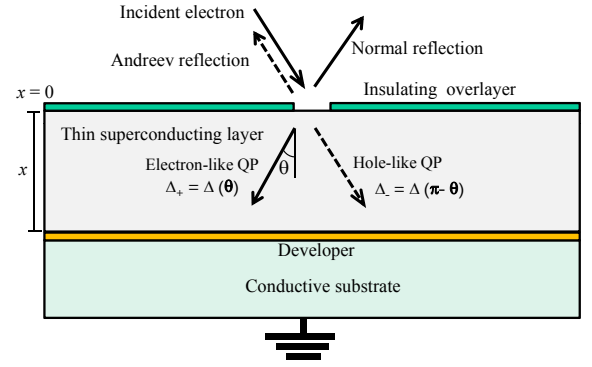


FIG. 1. (Color online) Schematic illustration of the Fresnel single aperture diffraction experiment for a thin superconductor layer (with thickness x). Reflection and transmission processes of a NIS tunnelling junction are shown. The developer is where the diffraction pattern is recorded.

tor, is grown firstly. Next, a sheet of electron-density sensitive developer for recording the diffraction pattern is deposited. The developer can be made either by the electron-sensitive material (like the photographic film) or alternatively by the fluorescent material (like the TV screen). On top of the recording sheet, a thin layer of SC single crystal with desired orientation and thickness is assembled. The last step is to coat an insulating layer on the thin SC layer with a small circular aperture (by mechanical and/or optical method) for electron beam injection. While electron beam can be made by natural radioactivity or low-energy accelerator, it can be alternatively due to a sharp conductive STM tip by an applied voltage bias. For the latter case, an insulating layer is not needed because the separation between the tip and the SC thin layer already acts like an insulating layer between it.

When electrons tunnel into the superconductor through the circular aperture, matter waves can interfere constructively or destructively. With enough electrons

passing through, clear diffraction pattern can be recorded in the developer while extra electrons will flow into the ground (see Fig. 1). To maintain the coherence for the FSAD signal, the thickness of the thin SC layer should be made comparable to the SC coherence length. Moreover, quasiparticles needs to be in the ballistic transport regime or the signal will be less clear. Scanning tunneling spectroscopy and vortex imaging have revealed that iron-pnictide superconductors have a short coherence length, $\xi \approx 27.6 \pm 2.9 \text{ \AA}$ [18], comparable to that of cuprate superconductors ($\xi \leq 20 \text{ \AA}$) [19]. Nevertheless, modern film growing technique has recently advanced that by improving the quality of the substrate which minimizes the inverse proximity effect, a nearly perfect ultrathin high- T_c SC layer can be grown as thin as three unit cells only [20]. This makes the proposed FSAD experiment feasible.

Quasiparticle (QP) states of an inhomogeneous superconductor have a coupled electron-hole character and can be described by the BdG equations [21]

$$\begin{aligned} E_{\mathbf{k}} u &= h_0 u + \Delta_{\mathbf{k}} v \\ E_{\mathbf{k}} v &= \Delta_{\mathbf{k}}^* u - h_0 v, \end{aligned} \quad (1)$$

where $h_0 \equiv -\hbar^2 \nabla^2 / 2m - \mu$ with μ the chemical potential and m the electron mass. We consider the quantum tunneling in an NIS junction where the thin SC layer is made normal to the x -axis and the pairing potential is assumed to be $\sim \Delta_{\mathbf{k}} \Theta(x)$ with $\Theta(x)$ the Heaviside step function and $\Delta_{\mathbf{k}}$ the SC gap function in the momentum space [22]. For simplicity, proximity effect of the SC order parameter is ignored at the interface. Under the WKBJ approximation [23], QP wavefunctions for the SC thin layer side ($x > 0$) are

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} e^{i\mathbf{k}_F \cdot \mathbf{r}} \tilde{u} \\ e^{-i\mathbf{k}_F \cdot \mathbf{r}} \tilde{v} \end{pmatrix} \text{ and } \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = e^{-\gamma x} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}, \quad (2)$$

where $\mathbf{k}_F \equiv (k_x, \mathbf{k}_{\parallel})$ is the Fermi wavevector and γ is the attenuation constant. With Eq. (2), Eq. (1) can be reduced to the Andreev equation

$$E_{\mathbf{k}} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix} = \begin{pmatrix} \varepsilon & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & -\varepsilon \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}, \quad (3)$$

where $\varepsilon \equiv i\gamma k_x / m$. The wavevector parallel to the interface, \mathbf{k}_{\parallel} , is conserved during the processes [24].

Solving Eq. (3), one obtains two degenerate eigenstates corresponding respectively to electron- and hole-like QPs:

$$\psi_{\mathbf{k}}^e(\mathbf{r}) = \begin{pmatrix} \Delta_+ \\ E_{\mathbf{k}} - \varepsilon \end{pmatrix} e^{i\mathbf{k}_F \cdot \mathbf{r}}; \quad \psi_{\mathbf{k}}^h(\mathbf{r}) = \begin{pmatrix} E_{\mathbf{k}} + \varepsilon \\ \Delta_- \end{pmatrix} e^{-i\mathbf{k}_F \cdot \mathbf{r}}, \quad (4)$$

where $E_{\mathbf{k}} = \sqrt{\Delta_+^2 + \varepsilon^2}$, $\Delta_+ \equiv \Delta(k_x, \mathbf{k}_{\parallel}) = \Delta(\theta)$, and $\Delta_- \equiv \Delta(-k_x, \mathbf{k}_{\parallel}) = \Delta(\pi - \theta)$ (scattering angle θ is defined in Fig. 1). Superposition of the above two eigenstates will give a resulting wave function for the SC layer

$$\psi_S(\mathbf{r}) = e^{-\gamma x} [c_1 \psi_{\mathbf{k}}^e(\mathbf{r}) + c_2 \psi_{\mathbf{k}}^h(\mathbf{r})]. \quad (5)$$

The coefficients c_1 and c_2 are important which are to be determined by the boundary conditions. Apart from the factor $e^{-\gamma x}$, Eqs. (2)–(5) give explicitly

$$\begin{aligned} \hat{u}(\mathbf{r}) &= c_1 \Delta_+ e^{i\mathbf{k}_F \cdot \mathbf{r}} + c_2 (E_{\mathbf{k}} + \varepsilon) e^{-i\mathbf{k}_F \cdot \mathbf{r}}, \\ \hat{v}(\mathbf{r}) &= c_1 (E_{\mathbf{k}} - \varepsilon) e^{i\mathbf{k}_F \cdot \mathbf{r}} + c_2 \Delta_- e^{-i\mathbf{k}_F \cdot \mathbf{r}}. \end{aligned} \quad (6)$$

When an electron is injected into the SC layer through the aperture, there are two types of reflections: normal reflection of electrons (with the coefficient r_N) and Andreev reflection of holes (with the coefficient r_A). In terms of r_N and r_A , the resulting wave function for the normal side ($x < 0$) can be written as

$$\psi_N(\mathbf{r}) = \begin{bmatrix} e^{i\mathbf{k}_F \cdot \mathbf{r}} + r_N e^{-i\mathbf{k}_F \cdot \mathbf{r}} \\ r_A e^{i\mathbf{k}_F \cdot \mathbf{r}} \end{bmatrix}. \quad (7)$$

By applying the following boundary conditions:

$$\begin{aligned} \psi_N(\mathbf{r})|_{x=0^-} &= \psi_S(\mathbf{r})|_{x=0^+}, \\ \frac{2mH}{\hbar^2} \psi_S(\mathbf{r})|_{x=0^+} &= \frac{d\psi_S(\mathbf{r})}{dz}|_{x=0^+} - \frac{d\psi_N(\mathbf{r})}{dz}|_{x=0^-} \end{aligned} \quad (8)$$

with H the height of the delta-function potential for the barrier, coefficients in (6) are solved to be $c_1 = \Delta_- (1 - iZ)/D$ and $c_2 = iZ(E_{\mathbf{k}} + \varepsilon)/D$ with $D = \Delta_+ \Delta_- (1 + Z^2) - Z^2(E_{\mathbf{k}} - \varepsilon)^2$ and $Z \equiv 2mH/\hbar^2 k_F$ being the effective potential barrier.

In general, the diffraction pattern recorded in the developer will be proportional to the QP density developed on it. In the current case, the FSAD intensity is proportional to

$$I(\mathbf{r}) = \frac{1}{S} \sum_{i, \mathbf{k}} \left[|\hat{u}_i(\mathbf{r})|^2 f(E_{\mathbf{k}}) + |\hat{v}_i(\mathbf{r})|^2 f(-E_{\mathbf{k}}) \right] \Delta S_i, \quad (9)$$

where $f(E_{\mathbf{k}}) = (e^{\beta E_{\mathbf{k}}} + 1)^{-1}$ and considering the size effect, a spatial average over the aperture (of area S) is taken where ΔS_i denotes a tiny cell within S .

Gap symmetry and barrier Z dependent FSAD – For simplicity, we shall consider the limit such that aperture diameter d is much smaller than the thickness x of the SC layer. This means that the spatial average in (9) is not needed. In the limit of $T \rightarrow 0$, interesting results of SC gap symmetry and barrier Z dependent FSAD will be obtained. Knowing the coefficients c_1 and c_2 , QP wavefunctions developed at $\mathbf{r} = (x, 0, 0)$ on the developer are obtained to be

$$\begin{aligned} \hat{u}(x) &= \hat{v}(x) \\ &= \begin{cases} e^{ik_x x} - 2iZ \sin(k_x x), & \text{if } \Delta_- = \Delta_+ \\ e^{ik_x x} - 2iZ \cos(k_x x), & \text{if } \Delta_- = -\Delta_+ \end{cases} \end{aligned} \quad (10)$$

There are many observable consequences out of the above symmetry-dependent results. In the following, we illuminate how one can probe the pairing symmetry and Fermi surface of a superconductor based on Eq. (10).

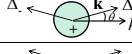




	symmetry/geometry	zero-order FSAD
s		$\Delta_- = \Delta_+$ min
p_x		$\Delta_- = -\Delta_+$ max
p_y		$\Delta_- = \Delta_+$ min
$d_{x^2-y^2}$		$\Delta_- = \Delta_+$ min
d_{xy}		$\Delta_- = -\Delta_+$ max

FIG. 2. (Color online) Illustration of SC gap symmetry dependent FSAD in the large- Z limit.

When barrier is low, $Z \ll 1$, $\hat{u}(x) = \hat{v}(x) = \exp(ik_x x)$ for both even ($\Delta_- = \Delta_+$) and odd ($\Delta_- = -\Delta_+$) symmetries. In this limit, FSAD pattern recorded in the developer makes no difference between the two symmetries. In this case, $I = 1$ and a zeroth-order maximum FSAD pattern (Airy disk) will occur. Nevertheless, the $Z \ll 1$ FSAD pattern can be used to measure the FS of the SC sample. Using the well-known formula $\sin \theta = 1.22\lambda/d$ (d is the aperture diameter) that locates first minimum of the Airy pattern, one can measure θ which determines the de Broglie wavelength of electrons, λ , and hence unambiguously identify the Fermi vector along the particular direction via the relation, $k_x = 2\pi/\lambda$. It should be emphasized that the above result remains valid even when Z is not too small ($Z \lesssim 1$).

Of most interest is when the barrier is high, $Z \gg 1$, to which *only the first Fresnel zone appears when d is small enough*. In this limit, $\hat{u}(x) = \hat{v}(x) \sim \sin(k_x x)$ for even symmetry and $\sim \cos(k_x x)$ for odd symmetry. Consequently

$$I \sim \begin{cases} \sin^2(k_x x), & \text{if } \Delta_- = \Delta_+ \\ \cos^2(k_x x), & \text{if } \Delta_- = -\Delta_+ \end{cases} \quad (11)$$

and the zeroth-order FSAD pattern developed behaves drastically different between the two symmetries. Experimentally to create a high barrier Z a thin insulating layer can be coated on the SC layer in assembling the FSAD apparatus. Alternatively, Z can be tuned by adding a bias voltage in the substrate layer relative to the ground, in addition to the bias voltage between the tip and the substrate layer. Moreover, for the large- Z limit, it is well-known that for even-parity pairing, maximum conductance occurs when incident electron energy equals the gap amplitude, $E \approx \Delta$. While for odd-parity pairing, owing to the zero-bias bound (midgap) state, maximum conductance occurs at $E \approx 0$ [24]. Thus for the present FSAD experiment, one can try to tune the incident electron energy to gain maximum-intensity signal.

Knowing the Fermi vector k_x (at particular direction), one may grow the SC film for the FSAD experiment with the desired thickness x which satisfies $k_x x = n\pi$ (n is an integer) and is comparable to the coherence length ξ .

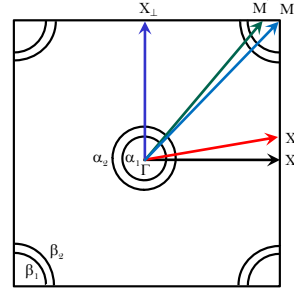


FIG. 3. (Color online) Schematic of the Fermi surfaces of Fe-pnictide superconductors in folded Brillouin zone. Important incident electron directions for FSAD experiment are shown.

Consequently for even symmetry, $I \sim \sin^2 \pi$ and FSAD will show a zeroth-order *minimum* at the developer. In contrast, for odd symmetry, $I \sim \cos^2 \pi$ and the FSAD will show a zeroth-order *maximum*.

Fig. 2 illustrates the large- Z gap-symmetry dependent FSAD pattern for different symmetries. While iron-pnictides seem to be spin-singlet superconductors with possibly s - and/or d -wave pairing symmetries [10], for completeness and for references to a spin-triplet superconductor of interest, we have also considered the cases of p -wave symmetry in Fig. 2 (and also in Table I). As is shown, for all cases we consider that the direction of injected electron, \mathbf{k} , is pointing near the k_x axis (with an angle θ). For s -wave gap, $\Delta_- = \Delta_+$ and the corresponding FSAD will be a zeroth-order minimum, which is apparently independent of the direction of electron injected. However, for nodal superconductors such as p - and d -wave cases, the results are two folds. If \mathbf{k} is pointing such that $\Delta_- = \Delta_+$ (for example the p_y and $d_{x^2-y^2}$ symmetries in Fig. 2), the corresponding FSAD will show a zeroth-order minimum. In contrast, if \mathbf{k} is pointing such that $\Delta_- = -\Delta_+$ (for example the p_x and d_{xy} symmetries in Fig. 2), the corresponding FSAD will show a zeroth-order maximum. It is worth noting that for all p - and d -wave nodal cases, if \mathbf{k} is pointing right at the nodes, $\Delta_+ = \Delta_- = 0$, the corresponding FSAD pattern will show a zeroth-order maximum, analogous to the case of a normal metal.

Moreover, for both $d_{x^2-y^2}$ and d_{xy} symmetries, zeroth-order FSAD pattern could change from maximum (minimum) to minimum (maximum) if the SC layer is grown with $\pi/4$ rotated about the c -axis (assuming that SC gap mainly develops in the ab plane). Similarly, for both p_x and p_y symmetries, zeroth-order FSAD pattern could change from maximum (minimum) to minimum (maximum) if the SC layer is grown with $\pi/2$ rotated about the c -axis. This gives another machinery for FSAD to distinguish between s -, p -, and d -wave pairing symmetries.

We now discuss possible schemes of FSAD patterns for multiband iron-pnictide superconductors. The so-called α sheets are concentric and nearly circular hole pockets around the Γ point. While the β sheets are nearly circular

TABLE I. Possible FSAD patterns for various pairing symmetries and incident directions shown in Fig. 3.

symmetry	ΓX	$\Gamma X'$	ΓM	$\Gamma M'$	ΓX_{\perp}
s	min	min	min	min	min
p_x	max	max	max	max	max
p_y	max	min	min	min	min
$d_{x^2-y^2}$	min	min	max	min	min
d_{xy}	max	max	max	max	max

electron pockets around the M points [25, 26]. These FS sheets are sketched in Fig. 3. If the pairing originates from the same mechanism, most likely α_1 and α_2 bands will have the same pairing symmetry. Similarly β_1 and β_2 bands will also likely have the same pairing symmetry. However, pairing symmetries may differ between α and β bands. Among other experiments, one can actually perform FSAD experiment to test the pairing symmetry of each *individual* band by carefully tuning the energy of incident electrons for maximum intensity with desired orientation and layer thickness.

More explicitly, one can first grow a set of thin layers with different crystal directions, and then perform small-Z FSAD experiments to measure and compile the FSs. With the knowing FSs, one can grow another set of thin layers with desired thickness x and crystal directions. For instance, if one thin layer has x simultaneously satisfying $k_1x = n_1\pi$ and $k_2x = n_2\pi$ with n_1, n_2 both integers and k_1 and k_2 the corresponding Fermi vectors of α_1 and α_2 (or β_1 and β_2) bands, one can then perform large-Z FSAD experiment on this thin layer to sort out the pairing symmetry on α and/or β bands. Taking $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ as an example, if $k_x \simeq 0.22\pi/a$ for β -band with lattice constant $a \simeq 0.4\text{nm}$ [27, 28], the thickness of the SC film can be better taken to be $x = n\pi/k_x \simeq n(4.55a) \simeq n(1.84\text{nm})$. For $n = 2$, $x \simeq 3.68\text{nm} = 36.8\text{\AA}$.

In Fig. 3, important directions of incident electrons of FSAD experiment are indicated for iron-pnictides. Possible FSAD patterns for various incident directions and pairing symmetries are listed in Table I. Note that it is also important to do the FSAD experiment for the $\Gamma X'$ and $\Gamma M'$ directions which are slightly deviated from the ΓX and ΓM directions. In view of Table I, if the zeroth-order FSAD pattern changes from maximum for ΓX to minimum for $\Gamma X'$ direction, pairing symmetry is likely to be p_y -wave. Similarly, it is likely to be $d_{x^2-y^2}$ -wave if it changes from maximum for ΓM to minimum for $\Gamma M'$ direction.

The proposed FSAD experiment is sensitive to the pairing gap symmetry on one particular FS. Due to the nature of a zero momentum transfer probe, it cannot link the pairing gap symmetries on two distant FSs. For iron-pnictides, one can use the experiment to check whether

it's s -wave on both α and β bands which is consistent with the s_{\pm} state, or s -wave on one band and d -wave on the other band. However, it is not able to tell if there is a sign change between the two bands. To verify the sign change, other experiments which can link the pairing symmetries on two distant FSs are in demand.

In summary, we propose that Fresnel single aperture diffraction (FSAD) could be a useful phase-sensitive probe for the pairing symmetry of a superconductor. It is demonstrated that FSAD pattern is intimately related to the SC pairing symmetry and the direction of incident electrons. Possible designs of FSAD experiment are suggested and discussed for iron-pnictide superconductors of complex multiple Fermi surface pairings. It is noted that the same scheme discussed in the present paper can also be applied to other phase-sensitive experiments, such as Young's interference and Fresnel lens.

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